

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037108.D
 Acq On : 27 Aug 2024 23:47
 Operator : SY/MD
 Sample : P3693-10
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K71

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M

Title : VOC Analysis

Signal : TIC: VV037108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.175	34	42	59	rBV	73643	159233	7.03%	0.910%
2	1.278	68	74	88	rVB	253891	270158	11.92%	1.544%
3	1.529	146	152	167	rVB	226389	272685	12.03%	1.559%
4	2.056	308	316	329	rVB	487517	690970	30.49%	3.950%
5	3.339	713	715	720	rBV6	1429	1161	0.05%	0.007%
6	3.680	819	821	824	rBV4	869	393	0.02%	0.002%
7	3.709	828	830	833	rVB4	1158	646	0.03%	0.004%
8	3.799	848	858	892	rBV2	180235	519128	22.90%	2.967%
9	4.243	981	996	1023	rBV2	357245	898889	39.66%	5.138%
10	4.481	1068	1070	1073	rBV4	1001	550	0.02%	0.003%
11	4.555	1091	1093	1096	rBV5	745	378	0.02%	0.002%
12	4.609	1109	1110	1113	rBV3	729	398	0.02%	0.002%
13	4.642	1118	1120	1122	rBV2	1107	662	0.03%	0.004%
14	4.735	1146	1149	1151	rVB3	1143	534	0.02%	0.003%
15	4.773	1159	1161	1164	rBV2	1026	572	0.03%	0.003%
16	4.805	1168	1171	1172	rBV3	956	470	0.02%	0.003%
17	4.828	1177	1178	1179	rBV2	470	155	0.01%	0.001%
18	4.889	1195	1197	1199	rBV3	955	518	0.02%	0.003%
19	4.950	1200	1216	1245	rBV2	903594	2266543	100.00%	12.956%
20	5.529	1383	1396	1430	rBV	729646	1514476	66.82%	8.657%
21	5.986	1524	1538	1567	rBV	510371	1048860	46.28%	5.995%
22	6.310	1635	1639	1643	rBV5	2203	1950	0.09%	0.011%
23	6.378	1658	1660	1661	rBV2	722	289	0.01%	0.002%
24	6.404	1666	1668	1670	rBV4	1237	587	0.03%	0.003%
25	6.503	1697	1699	1701	rBV3	578	192	0.01%	0.001%
26	6.519	1701	1704	1710	rVB7	1156	1302	0.06%	0.007%
27	6.545	1710	1712	1714	rBV3	887	411	0.02%	0.002%
28	6.558	1714	1716	1717	rBV2	685	258	0.01%	0.001%
29	6.606	1730	1731	1732	rBV2	867	284	0.01%	0.002%
30	6.690	1755	1757	1760	rBV4	1312	927	0.04%	0.005%
31	6.764	1777	1780	1784	rVB4	1499	1181	0.05%	0.007%
32	6.786	1784	1787	1789	rVB4	939	584	0.03%	0.003%
33	6.857	1807	1809	1811	rBV3	1103	569	0.03%	0.003%
34	6.912	1816	1826	1859	rBV2	240973	470370	20.75%	2.689%
35	7.239	1916	1928	1957	rBV	1013701	1794820	79.19%	10.259%
36	7.551	2015	2025	2052	rBV	157857	300009	13.24%	1.715%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
 Data File : VV037108.D
 Acq On : 27 Aug 2024 23:47
 Operator : SY/MD
 Sample : P3693-10
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 E1K71

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
 Title : VOC Analysis

37	7.770	2091	2093	2096	rBV5	1352	651	0.03%	0.004%
38	7.973	2153	2156	2157	rBV3	1676	794	0.04%	0.005%
39	8.027	2164	2173	2206	rBV	419393	842928	37.19%	4.818%
40	8.683	2370	2377	2378	rBV7	1741	1819	0.08%	0.010%
41	8.780	2392	2407	2434	rBV	1109896	1851741	81.70%	10.585%
42	9.214	2538	2542	2544	rBV6	2278	1510	0.07%	0.009%
43	9.374	2590	2592	2594	rBV3	1343	549	0.02%	0.003%
44	9.410	2601	2603	2606	rBV5	1044	554	0.02%	0.003%
45	9.429	2606	2609	2610	rBV3	1123	671	0.03%	0.004%
46	9.490	2621	2628	2633	rBV3	1758	2525	0.11%	0.014%
47	9.532	2636	2641	2645	rBV7	2199	2013	0.09%	0.012%
48	9.567	2650	2652	2655	rVB4	795	348	0.02%	0.002%
49	9.651	2675	2678	2682	rBV5	1138	1013	0.04%	0.006%
50	9.709	2694	2696	2697	rBV2	691	269	0.01%	0.002%
51	9.763	2710	2713	2716	rBV5	1113	680	0.03%	0.004%
52	9.812	2721	2728	2730	rBV7	1465	1314	0.06%	0.008%
53	9.863	2740	2744	2747	rBV5	1143	965	0.04%	0.006%
54	9.892	2751	2753	2760	rBV7	994	1116	0.05%	0.006%
55	10.024	2791	2794	2796	rBV3	924	710	0.03%	0.004%
56	10.098	2812	2817	2819	rBV5	1442	1379	0.06%	0.008%
57	10.149	2821	2833	2856	rVV	665165	1055767	46.58%	6.035%
58	10.403	2910	2912	2915	rVB4	1116	485	0.02%	0.003%
59	10.464	2926	2931	2932	rBV5	1234	917	0.04%	0.005%
60	10.561	2959	2961	2963	rBV3	817	485	0.02%	0.003%
61	10.619	2976	2979	2982	rVB4	1075	598	0.03%	0.003%
62	10.644	2985	2987	2992	rVB4	1267	685	0.03%	0.004%
63	10.664	2992	2993	2995	rBV2	1014	508	0.02%	0.003%
64	10.699	2999	3004	3009	rVB5	1791	1928	0.09%	0.011%
65	10.722	3009	3011	3014	rBV3	1270	769	0.03%	0.004%
66	10.735	3014	3015	3018	rBV3	895	399	0.02%	0.002%
67	10.815	3038	3040	3043	rVB4	1305	650	0.03%	0.004%
68	10.853	3049	3052	3055	rBV5	1065	772	0.03%	0.004%
69	10.950	3078	3082	3083	rBV4	808	511	0.02%	0.003%
70	10.992	3094	3095	3098	rBV2	764	383	0.02%	0.002%
71	11.030	3104	3107	3108	rBV2	890	529	0.02%	0.003%
72	11.072	3118	3120	3121	rBV	603	229	0.01%	0.001%
73	11.114	3131	3133	3134	rBV3	1051	457	0.02%	0.003%
74	11.181	3143	3154	3178	rBV	1146815	1824619	80.50%	10.430%
75	11.554	3259	3270	3297	rBV	1038789	1653049	72.93%	9.449%
76	12.014	3410	3413	3414	rBV2	1009	678	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037108.D
Acq On : 27 Aug 2024 23:47
Operator : SY/MD
Sample : P3693-10
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K71

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M

Title : VOC Analysis

77	12.249	3484	3486	3490	rBV5	1128	644	0.03%	0.004%
78	12.384	3524	3528	3529	rBV3	1396	1074	0.05%	0.006%
79	12.461	3550	3552	3555	rBV4	1288	693	0.03%	0.004%
80	12.548	3573	3579	3580	rBV3	1478	1498	0.07%	0.009%
81	12.651	3608	3611	3616	rVB5	1562	1120	0.05%	0.006%
82	13.014	3723	3724	3727	rVB2	1648	612	0.03%	0.003%
83	13.448	3853	3859	3860	rBV5	1895	1479	0.07%	0.008%
84	13.593	3900	3904	3907	rBV4	1705	1476	0.07%	0.008%
85	13.641	3916	3919	3923	rBV5	1858	1754	0.08%	0.010%
86	13.841	3979	3981	3983	rBV4	1126	505	0.02%	0.003%
87	14.059	4047	4049	4051	rBV3	967	396	0.02%	0.002%
88	14.181	4084	4087	4090	rBV6	1562	1220	0.05%	0.007%
89	14.300	4122	4124	4128	rBV4	1475	1142	0.05%	0.007%
90	14.464	4172	4175	4177	rBV4	2181	1723	0.08%	0.010%

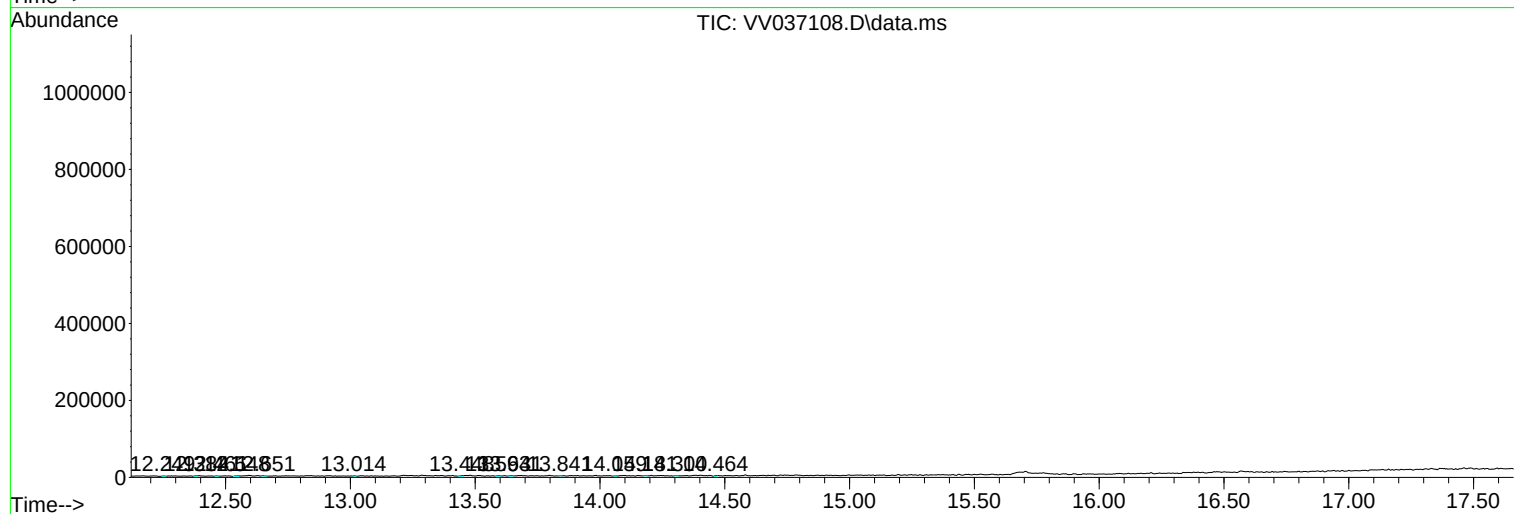
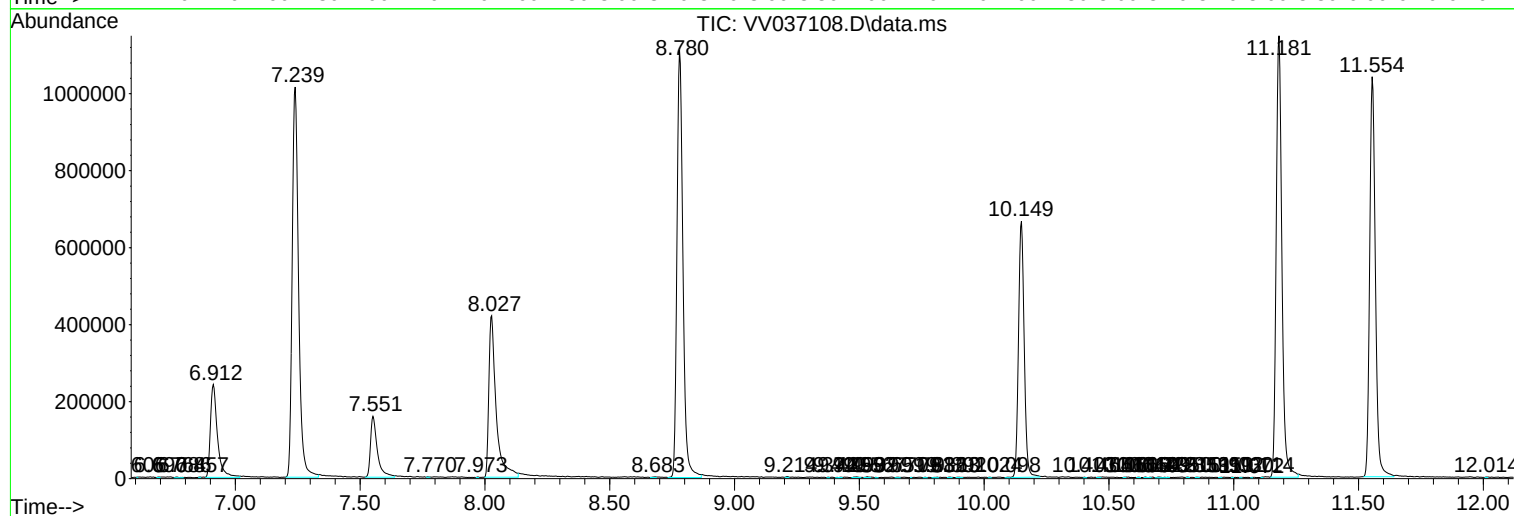
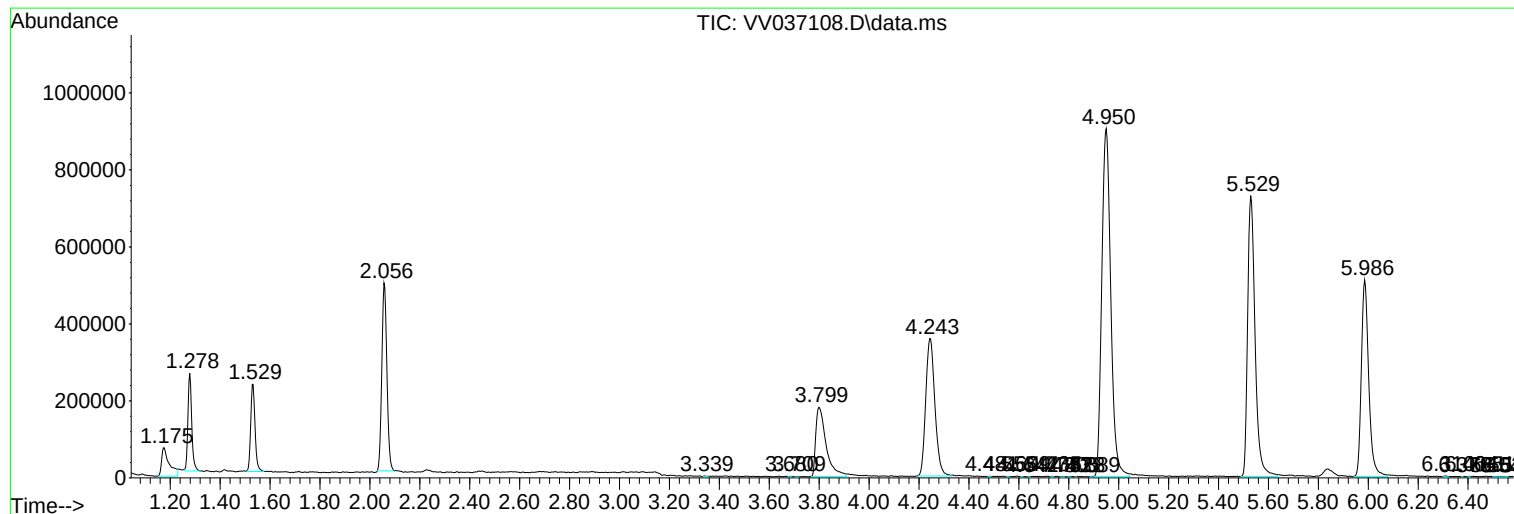
Sum of corrected areas: 17494415

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037108.D
Acq On : 27 Aug 2024 23:47
Operator : SY/MD
Sample : P3693-10
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037108.D
Acq On : 27 Aug 2024 23:47
Operator : SY/MD
Sample : P3693-10
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K71

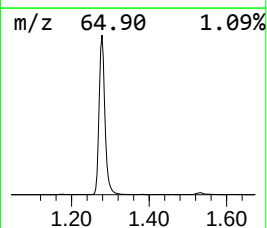
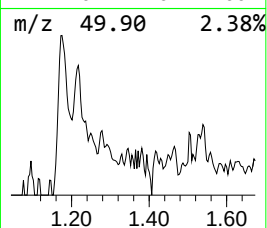
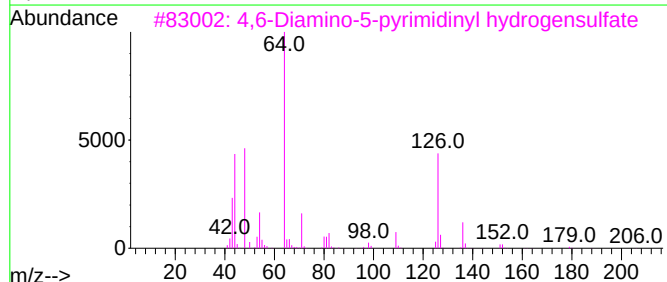
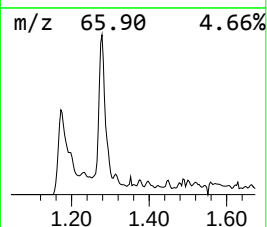
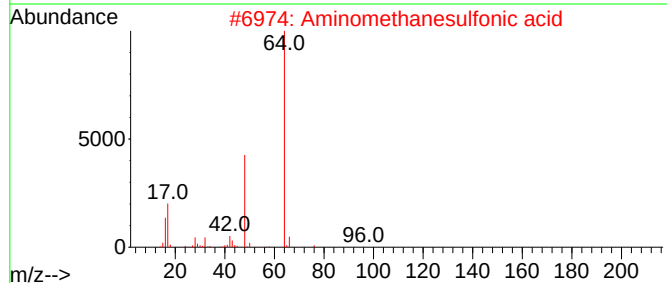
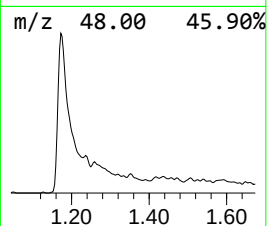
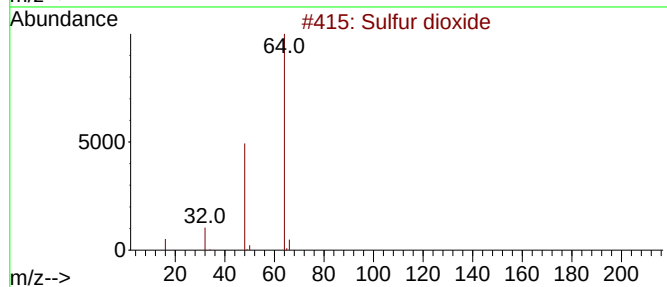
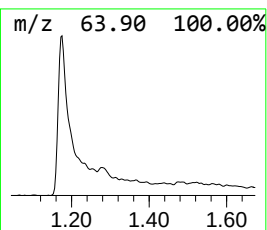
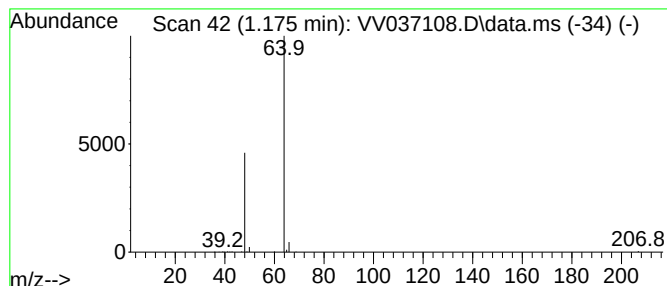
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.175	5.26 ug/L	159233	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9
4			Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082724\
Data File : VV037108.D
Acq On : 27 Aug 2024 23:47
Operator : SY/MD
Sample : P3693-10
Misc : 5.00mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E1K71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.175	5.3	ug/L	159233	1	5.529	1514480	50.0